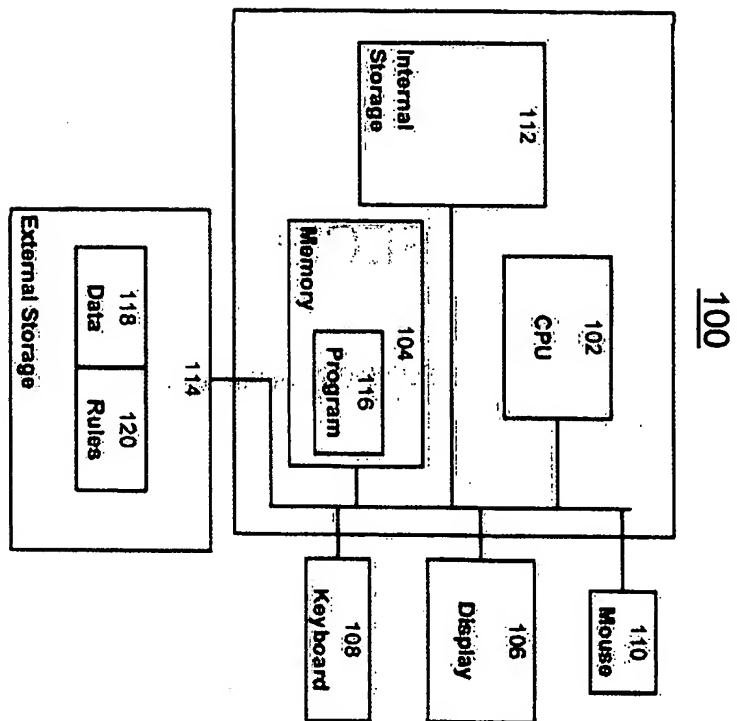




Fig. 1



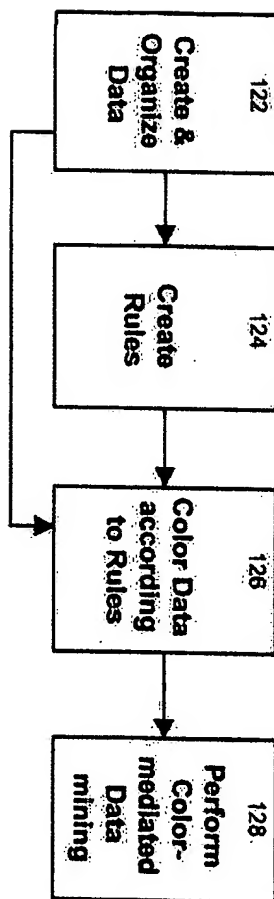


Fig. 2



Microsoft Excel - demo PATENT 10-48022-1.mt - Head Print									
A1									
Cmpd									
Cmpd	Series	Test1	Test2	Test3	HTS SPA Dose-Resp % inh @ 3x10-6M	HTS SPA Dose-Resp % inh @ 1x10-6M	HTS SPA Dose-Resp % inh @ 3x10-7M	HTS SPA Dose-Resp % inh @ 1x10-7M	
Cmpd1	N		28	30	41	3	22	6	
Cmpd2	N		42	65	83	57	28	16	
Cmpd3	G		261	11	70	26	24	28	
Cmpd4	N			30	89	60	21	22	
Cmpd5	N		18	32	71	41	13	3	
Cmpd6	D	8.86	6.5	32	100	79	48	49	
Cmpd7	D	3.11	0.037	7.8	68	26	28	38	
Cmpd8	D		0.088	2.6	68	41	22	16	
Cmpd9	D	0.119			61	42	24	5	
Cmpd10	N	0.233			50	77	63	26	
Cmpd11	N	4.31			47	25	24	3	
Cmpd12	H	1.3	0.24		91	39	40	37	
Cmpd13	H	1.17	0.194	30	29	23	4	12	
Cmpd14	H	0.28	0.41		89	46	46	36	
Cmpd15	H	0.369	0.146		101	82	38	18	
Cmpd16	I		0.87	30	81	64	47	24	
Cmpd17	K		0.223	30	79	54	22	22	
Cmpd18	I	6.27			71	71	23	12	
Cmpd19	I	0.134			101	109	108	100	
Cmpd20	F		0.917		87	70	31	13	
Cmpd21	K		2.21		94	77	36	12	
Cmpd22	B		0.16		98	61	36	12	
Cmpd23	B				110	91	69	39	
Cmpd24	B		0.27		100	104	75	52	
Cmpd25	B	0.041	1.1		93	71	41	22	
Cmpd26	B	0.685			97	79	43	23	
Cmpd27	B	0.111			96	93	62	26	
Cmpd28	E		0.13		69	62	12	11	
Cmpd29	J		0.46		41	40	9	17	
Cmpd30	J	2.78	46						

302 304 306 308 310 312 314

Fig. 3A

Cirpd	Series	Test1	Test2	Test3	HTS SPA Dose-Resp % Inhib @ 3x10 ⁻⁶ M	HTS SPA Dose-Resp % Inhib @ 1x10 ⁻⁵ M	HTS SPA Dose-Resp % Inhib @ 3x10 ⁻⁷ M	HTS SPA Dose-Resp % Inhib @ 1x10 ⁻⁷ M
Cmpd41	J	227	24	30	106	62	18	3
Cmpd45	J	0.63			44	28		
Cmpd46	J		0.23		50	63	42	14
Cmpd47	N	12.3			56	20	38	20
Cmpd48	L	0.009	0.024		50	50	51	2
Cmpd49	F	0.56	0.41		87	73	29	15
Cmpd40	G	0.268	1.04		65	66	40	11
Cmpd41	O	0.018	0.35		58	46	28	13
Cmpd42	F	0.38	0.9		102	87	32	87
Cmpd43	H	4.45	0.13		38	25	18	12
Cmpd44	G	0.076	0.1		78	60	40	25
Cmpd45	F	0.5			111	110	104	82
Cmpd46	M	1.14			25	21	16	21
Cmpd47	F	0.026			109	104	97	80
Cmpd48	F	0.22			100	102	83	75
Cmpd49	M	0.035	0.043		71	43	31	15
Cmpd50	F	0.051			112	111	112	75
Cmpd51	G	0.079			78	70	44	27
Cmpd52	H	0.23	0.117	4.9	69	24	23	14
Cmpd53	A	0.005	0.18	15	108	102	53	27
Cmpd54	A	0.33			91	78	76	33
Cmpd55	G	9.12			61	64	60	26
Cmpd56	C	0.29			93	80	55	37
Cmpd57	A	0.018			101	72	42	29
Cmpd58	C	0.22			92	69	55	49

Fig. 3B

130-1 — 140 — 130-2 132 134 136 138 142

[illegible]

Fig. 4A

Click here to run these	Click here to run these	Click here to run these	Click here to run these	Click here to run these	Click here to run these	Click here to run these
sheet DEMO 3 column(s) Bc # of colors 200 break 1 50 break 2 200 break 3 1,00E+05 break 4 color 1 color 2 color 3 color 4 Re-scale all? yes	sheet DEMO 3 column(s) Bc # of colors 200 break 1 50 break 2 200 break 3 1,00E+05 break 4 color 1 color 2 color 3 color 4 Re-scale all?	sheet DEMO 3 column(s) B/D # of colors 100000 break 1 no effect break 2 > 10000 break 3 effect, 10000 break 4 > 300 break 5 < 30 color 1 color 2 color 3 color 4 color 5 Re-scale all?	sheet DEMO 3 column(s) B/D # of colors 100000 break 1 no effect break 2 > 10000 break 3 no effect break 4 > 10000 break 5 color 1 color 2 color 3 color 4 color 5 Re-scale all?	sheet DEMO 3 column(s) 1,0E+05 # of colors 100000 break 1 break 2 break 3 break 4 break 5 color 1 color 2 color 3 color 4 color 5 color 6 Re-scale all?	sheet DEMO 3 column(s) 1,0E+05 # of colors 100000 break 1 break 2 break 3 break 4 break 5 color 1 color 2 color 3 color 4 color 5 color 6 Re-scale all?	sheet DEMO 3 column(s) 1,0E+05 # of colors 100000 break 1 break 2 break 3 break 4 break 5 color 1 color 2 color 3 color 4 color 5 color 6 Re-scale all?

Fig. 4B

Fig. 5A



Color Management	
Sheet	DEMO 1
column(s)	C,D
# of colors	4
break 1	0.1
break 2	1
break 3	5
break 4	
color 1	
color 2 yellow	
color 3 orange	
color 4 red	
Re-scale all?	no

Fig. 58



152

DEMO 3	
sheet	DEMO 3
column(s)	
# of colors	6
break 1	
break 2	
break 3	
break 4	
break 5	
color 1	
color 2	
color 3	
color 4	
color 5	
color 6	
Re-scale all?	

144

146

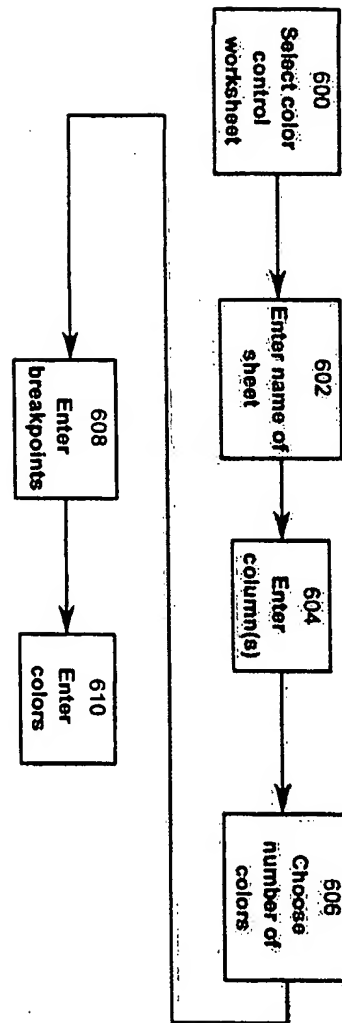
148

150

Fig. 6A



Fig. 6B



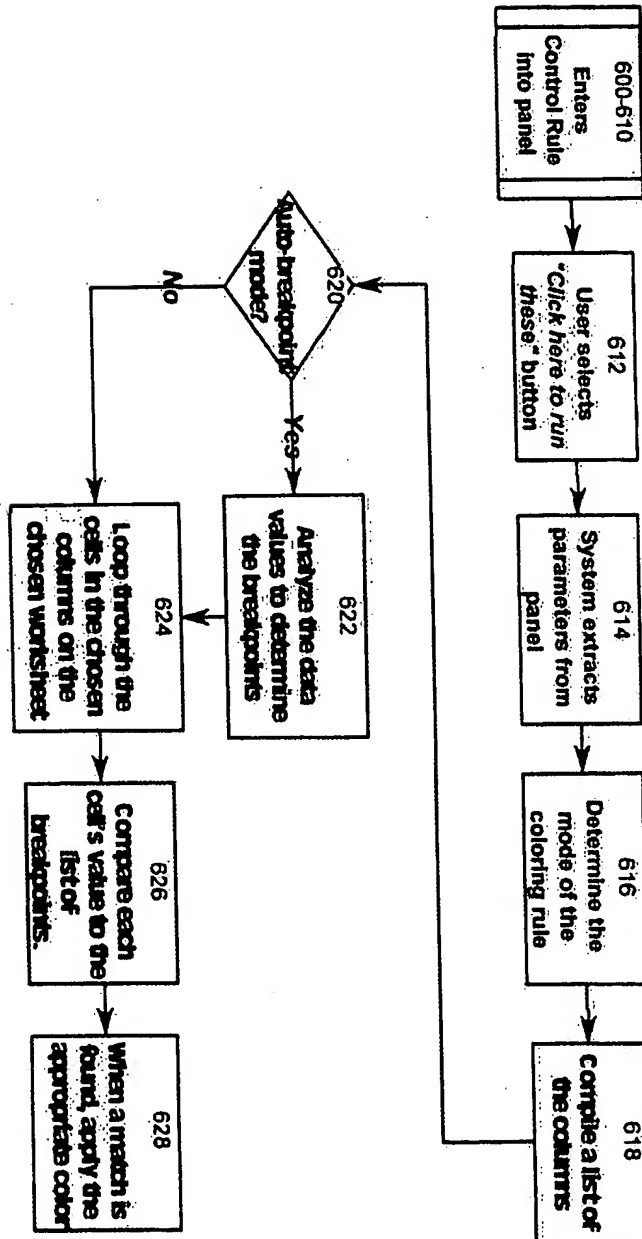


Fig. 6C



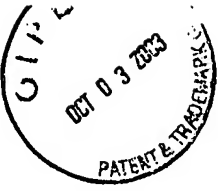
Compd	Series	Test1	Test2	Test3	HTS SPA Dose-Resp % Inhib @ 3x10-6M	HTS SPA Dose-Resp % Inhib @ 1x10-6M	HTS SPA Dose-Resp % Inhib @ 3x10-7M	HTS SPA Dose-Resp % Inhib @ 1x10-7M
Comp001	N		34	30	41	3	22	5
Comp002	N		42	11	83	57	28	15
Comp003	G		37.5	30	70	25	24	23
Comp004	N			32	88	60	21	22
Comp005	N			37	71	41	13	3
Comp006	D	9.55	4.5	78	100	79	48	43
Comp007	D	5.63	0.687	26	65	28	28	38
Comp008	D		0.055		68	41	22	15
Comp009	D	0.119			61	42	24	5
Comp010	N	0.220			50	77	63	25
Comp011	N	0.231			47	25	24	3
Comp012	H	0.24	0.24	30	81	59	40	37
Comp013	H	0.194	0.194		39	22	4	12
Comp014	H	0.26	0.41		89	46	46	36
Comp015	H	0.389	0.148	30	101	82	38	18
Comp016	I		0.87	30	81	64	47	24
Comp017	K		0.223		79	64	22	32
Comp018	I	4.27			71	71	23	12
Comp019	I	0.134			101	109	108	100
Comp020	F		0.217		87	70	31	12
Comp021	K		22.31		94	77	36	12
Comp022	B		0.15		96	61	36	12
Comp023	B				110	91	89	39
Comp024	B		0.27		105	104	75	52
Comp025	B				93	71	41	22
Comp026	B	0.850	0.06		97	79	43	23
Comp027	B	0.117			95	53	32	25
Comp028	E		0.13		68	62	12	11
Comp029	J		0.48		41	48	9	17
Comp030	J	5.5	1.6	5.2	5	6	21	8
Comp031	N				62	30	15	33
Comp032	J				112	29	75	14
Comp033	N				105	62	62	21
Comp034	J		24	30				

Fig. 7A

Fig. 7B

Compd	Series	Test1	Test2	Test3	HTS SPA Dose-Resp % inh @ 3x10 ⁻⁶ M	HTS SPA Dose-Resp % inh @ 1x10 ⁻⁶ M	HTS SPA Dose-Resp % inh @ 3x10 ⁻⁷ M	HTS SPA Dose-Resp % inh @ 1x10 ⁻⁷ M
Compd1	N		35	20				
Compd2	N		1	11	83	3	22	9
Compd3	G		10	20	70	26	21	16
Compd4	N				88	30	21	15
Compd5	N		45	37	71	27	13	22
Compd6	D	3.2E			10	79	11	18
Compd7	D	5.1E			10	79	11	18
Compd8	D			26	85	63	22	26
Compd9	D	0.119			89	63	22	15
Compd10	N	0.235			61	77	23	5
Compd11	N				20	32	23	25
Compd12	H	0.09	0.24		81	32	23	3
Compd13	H	0.194		30	81	32	23	12
Compd14	H	0.26	0.41		81	32	23	12
Compd15	H	0.363	0.448		81	32	23	12
Compd16	I		0.87	20	81	32	23	12
Compd17	K		0.223	30	81	32	23	12
Compd18	I	5.22			79	71	23	12
Compd19	I	0.124			79	71	23	12
Compd20	F		0.17		97	70	23	12
Compd21	K				97	70	23	12
Compd22	B		0.16		97	70	23	12
Compd23	B				97	70	23	12
Compd24	B		0.27		97	70	23	12
Compd25	B				97	70	23	12
Compd26	B	0.885			97	70	23	12
Compd27	B	0.111			97	70	23	12
Compd28	E		0.12		97	70	23	12
Compd29	J		0.40		97	70	23	12
Compd30	J		15		97	70	23	12
Compd31	N				97	70	23	12
Compd32	J				97	70	23	12
Compd33	N				97	70	23	12

Fig. 8A



USSN 10/048,022
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Sheet 15 of 64

Compd	Series	Test1	Test2	Test3	HTS SPA Dose-Resp % inh @ 3x10-5M	HTS SPA Dose-Resp % inh @ 1x10-5M	HTS SPA Dose-Resp % inh @ 3x10-7M	HTS SPA Dose-Resp % inh @ 1x10-7M
35	Compd35	J	0.03	0.03	10	62	62	31
36	Compd36	J	0.03	0.03	10	62	62	31
37	Compd37	J	0.03	0.03	10	62	62	31
38	Compd38	N	12.1	0.03	10	62	62	31
39	Compd39	L	0.03	0.03	10	62	62	31
40	Compd40	F	0.03	0.03	10	62	62	31
41	Compd41	G	0.03	0.03	10	62	62	31
42	Compd42	F	0.03	0.03	10	62	62	31
43	Compd43	H	0.03	0.03	10	62	62	31
44	Compd44	G	0.03	0.03	10	62	62	31
45	Compd45	F	0.03	0.03	10	62	62	31
46	Compd46	M	0.03	0.03	10	62	62	31
47	Compd47	F	0.03	0.03	10	62	62	31
48	Compd48	F	0.03	0.03	10	62	62	31
49	Compd49	M	0.03	0.03	10	62	62	31
50	Compd50	F	0.03	0.03	10	62	62	31
51	Compd51	G	0.03	0.03	10	62	62	31
52	Compd52	H	0.03	0.03	10	62	62	31
53	Compd53	A	0.03	0.03	10	62	62	31
54	Compd54	A	0.03	0.03	10	62	62	31
55	Compd55	G	0.03	0.03	10	62	62	31
56	Compd56	C	0.03	0.03	10	62	62	31
57	Compd57	A	0.03	0.03	10	62	62	31
58	Compd58	C	0.03	0.03	10	62	62	31
59	Compd59	C	0.03	0.03	10	62	62	31
60	Compd60	C	0.03	0.03	10	62	62	31
61	Compd61	C	0.03	0.03	10	62	62	31
62	Compd62	C	0.03	0.03	10	62	62	31
63	Compd63	C	0.03	0.03	10	62	62	31
64	Compd64	C	0.03	0.03	10	62	62	31
65	Compd65	C	0.03	0.03	10	62	62	31
66	Compd66	C	0.03	0.03	10	62	62	31
67	Compd67	C	0.03	0.03	10	62	62	31
68	Compd68	C	0.03	0.03	10	62	62	31
69	Compd69	C	0.03	0.03	10	62	62	31
70	Compd70	C	0.03	0.03	10	62	62	31
71	Compd71	C	0.03	0.03	10	62	62	31
72	Compd72	C	0.03	0.03	10	62	62	31
73	Compd73	C	0.03	0.03	10	62	62	31
74	Compd74	C	0.03	0.03	10	62	62	31
75	Compd75	C	0.03	0.03	10	62	62	31
76	Compd76	C	0.03	0.03	10	62	62	31
77	Compd77	C	0.03	0.03	10	62	62	31
78	Compd78	C	0.03	0.03	10	62	62	31
79	Compd79	C	0.03	0.03	10	62	62	31
80	Compd80	C	0.03	0.03	10	62	62	31
81	Compd81	C	0.03	0.03	10	62	62	31
82	Compd82	C	0.03	0.03	10	62	62	31
83	Compd83	C	0.03	0.03	10	62	62	31
84	Compd84	C	0.03	0.03	10	62	62	31
85	Compd85	C	0.03	0.03	10	62	62	31
86	Compd86	C	0.03	0.03	10	62	62	31
87	Compd87	C	0.03	0.03	10	62	62	31
88	Compd88	C	0.03	0.03	10	62	62	31
89	Compd89	C	0.03	0.03	10	62	62	31
90	Compd90	C	0.03	0.03	10	62	62	31
91	Compd91	C	0.03	0.03	10	62	62	31
92	Compd92	C	0.03	0.03	10	62	62	31
93	Compd93	C	0.03	0.03	10	62	62	31
94	Compd94	C	0.03	0.03	10	62	62	31
95	Compd95	C	0.03	0.03	10	62	62	31
96	Compd96	C	0.03	0.03	10	62	62	31
97	Compd97	C	0.03	0.03	10	62	62	31
98	Compd98	C	0.03	0.03	10	62	62	31
99	Compd99	C	0.03	0.03	10	62	62	31
100	Compd100	C	0.03	0.03	10	62	62	31

Fig. 8B



Fig. 9A									
Row	Col	Col	Col	Col	Col	Col	Col	Col	Col
1	1	2	3	4	5	6	7	8	9
10	10	11	12	13	14	15	16	17	18
20	20	21	22	23	24	25	26	27	28
30	30	31	32	33	34	35	36	37	38
40	40	41	42	43	44	45	46	47	48
50	50	51	52	53	54	55	56	57	58
60	60	61	62	63	64	65	66	67	68
70	70	71	72	73	74	75	76	77	78
80	80	81	82	83	84	85	86	87	88
90	90	91	92	93	94	95	96	97	98
100	100	101	102	103	104	105	106	107	108
110	110	111	112	113	114	115	116	117	118
120	120	121	122	123	124	125	126	127	128
130	130	131	132	133	134	135	136	137	138
140	140	141	142	143	144	145	146	147	148
150	150	151	152	153	154	155	156	157	158
160	160	161	162	163	164	165	166	167	168
170	170	171	172	173	174	175	176	177	178
180	180	181	182	183	184	185	186	187	188
190	190	191	192	193	194	195	196	197	198
200	200	201	202	203	204	205	206	207	208
210	210	211	212	213	214	215	216	217	218
220	220	221	222	223	224	225	226	227	228
230	230	231	232	233	234	235	236	237	238
240	240	241	242	243	244	245	246	247	248
250	250	251	252	253	254	255	256	257	258
260	260	261	262	263	264	265	266	267	268
270	270	271	272	273	274	275	276	277	278
280	280	281	282	283	284	285	286	287	288
290	290	291	292	293	294	295	296	297	298
300	300	301	302	303	304	305	306	307	308
310	310	311	312	313	314	315	316	317	318
320	320	321	322	323	324	325	326	327	328
330	330	331	332	333	334	335	336	337	338
340	340	341	342	343	344	345	346	347	348
350	350	351	352	353	354	355	356	357	358
360	360	361	362	363	364	365	366	367	368
370	370	371	372	373	374	375	376	377	378
380	380	381	382	383	384	385	386	387	388
390	390	391	392	393	394	395	396	397	398
400	400	401	402	403	404	405	406	407	408
410	410	411	412	413	414	415	416	417	418
420	420	421	422	423	424	425	426	427	428
430	430	431	432	433	434	435	436	437	438
440	440	441	442	443	444	445	446	447	448
450	450	451	452	453	454	455	456	457	458
460	460	461	462	463	464	465	466	467	468
470	470	471	472	473	474	475	476	477	478
480	480	481	482	483	484	485	486	487	488
490	490	491	492	493	494	495	496	497	498
500	500	501	502	503	504	505	506	507	508
510	510	511	512	513	514	515	516	517	518
520	520	521	522	523	524	525	526	527	528
530	530	531	532	533	534	535	536	537	538
540	540	541	542	543	544	545	546	547	548
550	550	551	552	553	554	555	556	557	558
560	560	561	562	563	564	565	566	567	568
570	570	571	572	573	574	575	576	577	578
580	580	581	582	583	584	585	586	587	588
590	590	591	592	593	594	595	596	597	598
600	600	601	602	603	604	605	606	607	608
610	610	611	612	613	614	615	616	617	618
620	620	621	622	623	624	625	626	627	628
630	630	631	632	633	634	635	636	637	638
640	640	641	642	643	644	645	646	647	648
650	650	651	652	653	654	655	656	657	658
660	660	661	662	663	664	665	666	667	668
670	670	671	672	673	674	675	676	677	678
680	680	681	682	683	684	685	686	687	688
690	690	691	692	693	694	695	696	697	698
700	700	701	702	703	704	705	706	707	708
710	710	711	712	713	714	715	716	717	718
720	720	721	722	723	724	725	726	727	728
730	730	731	732	733	734	735	736	737	738
740	740	741	742	743	744	745	746	747	748
750	750	751	752	753	754	755	756	757	758
760	760	761	762	763	764	765	766	767	768
770	770	771	772	773	774	775	776	777	778
780	780	781	782	783	784	785	786	787	788
790	790	791	792	793	794	795	796	797	798
800	800	801	802	803	804	805	806	807	808
810	810	811	812	813	814	815	816	817	818
820	820	821	822	823	824	825	826	827	828
830	830	831	832	833	834	835	836	837	838
840	840	841	842	843	844	845	846	847	848
850	850	851	852	853	854	855	856	857	858
860	860	861	862	863	864	865	866	867	868
870	870	871	872	873	874	875	876	877	878
880	880	881	882	883	884	885	886	887	888
890	890	891	892	893	894	895	896	897	898
900	900	901	902	903	904	905	906	907	908
910	910	911	912	913	914	915	916	917	918
920	920	921	922	923	924	925	926	927	928
930	930	931	932	933	934	935	936	937	938
940	940	941	942	943	944	945	946	947	948
950	950	951	952	953	954	955	956	957	958
960	960	961	962	963	964	965	966	967	968
970	970	971	972	973	974	975	976	977	978
980	980	981	982	983	984	985	986	987	988
990	990	991	992	993	994	995	996	997	998
1000	1000	1001	1002	1003	1004	1005	1006	1007	1008

Fig. 9A

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OCT 03 2003

Fig. 9B



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1	F2 A	F2 B	F2 C	F2 D	F2 E	F2 F	F2 G	F2 H	F2 I	F2 J	F2 K	F2 L	F2 M	F2 N	F2 O	F2 P	F2 Q	F2 R	F2 S	F2 T	F2 U	F2 V	F2 W	F2 X	F2 Y	F2 Z	F2 AA	F2 AB	F2 AC	F2 AD	F2 AE	F2 AF	F2 AG	F2 AH	F2 AI	F2 AJ	F2 AK	F2 AL	F2 AM	F2 AN	F2 AO	F2 AP	F2 AQ	F2 AR	F2 AS	F2 AT	F2 AU	F2 AV	F2 AW	F2 AX	F2 AY	F2 AZ	F2 BA	F2 BB	F2 BC	F2 BD	F2 BE	F2 BF	F2 BG	F2 BH	F2 BI	F2 BJ	F2 BK	F2 BL	F2 BM	F2 BN	F2 BO	F2 BP	F2 BQ	F2 BR	F2 BS	F2 BT	F2 BU	F2 BV	F2 BW	F2 BX	F2 BY	F2 BZ	F2 CA	F2 CB	F2 CC	F2 CD	F2 CE	F2 CF	F2 CG	F2 CH	F2 CI	F2 CJ	F2 CK	F2 CL	F2 CM	F2 CN	F2 CO	F2 CP	F2 CQ	F2 CR	F2 CS	F2 CT	F2 CU	F2 CV	F2 CW	F2 CX	F2 CY	F2 CZ	F2 DA	F2 DB	F2 DC	F2 DD	F2 DE	F2 DF	F2 DG	F2 DH	F2 DI	F2 DJ	F2 DK	F2 DL	F2 DM	F2 DN	F2 DO	F2 DP	F2 DQ	F2 DR	F2 DS	F2 DT	F2 DU	F2 DV	F2 DW	F2 DX	F2 DY	F2 DZ	F2 EA	F2 EB	F2 EC	F2 ED	F2 EE	F2 EF	F2 EG	F2 EH	F2 EI	F2 EJ	F2 EK	F2 EL	F2 EM	F2 EN	F2 EO	F2 EP	F2 EQ	F2 ER	F2 ES	F2 ET	F2 EU	F2 EV	F2 EW	F2 EX	F2 EY	F2 EZ	F2 FA	F2 FB	F2 FC	F2 FD	F2 FE	F2 FF	F2 FG	F2 FH	F2 FI	F2 FJ	F2 FK	F2 FL	F2 FM	F2 FN	F2 FO	F2 FP	F2 FQ	F2 FR	F2 FS	F2 FT	F2 FU	F2 FV	F2 FW	F2 FX	F2 FY	F2 FZ	F2 GA	F2 GB	F2 GC	F2 GD	F2 GE	F2 GF	F2 GG	F2 GH	F2 GI	F2 GJ	F2 GK	F2 GL	F2 GM	F2 GN	F2 GO	F2 GP	F2 GQ	F2 GR	F2 GS	F2 GT	F2 GU	F2 GV	F2 GW	F2 GX	F2 GY	F2 GZ	F2 HA	F2 HB	F2 HC	F2 HD	F2 HE	F2 HF	F2 HG	F2 HH	F2 HI	F2 HJ	F2 HK	F2 HL	F2 HM	F2 HN	F2 HO	F2 HP	F2 HQ	F2 HR	F2 HS	F2 HT	F2 HU	F2 HV	F2 HW	F2 HX	F2 HY	F2 HZ	F2 IA	F2 IB	F2 IC	F2 ID	F2 IE	F2 IF	F2 IG	F2 IH	F2 II	F2 IJ	F2 IK	F2 IL	F2 IM	F2 IN	F2 IO	F2 IP	F2 IQ	F2 IR	F2 IS	F2 IT	F2 IU	F2 IV	F2 IW	F2 IX	F2 IY	F2 IZ	F2 JA	F2 JB	F2 JC	F2 JD	F2 JE	F2 JF	F2 JG	F2 JH	F2 JI	F2 JJ	F2 JK	F2 JL	F2 JM	F2 JN	F2 JO	F2 JP	F2 JQ	F2 JR	F2 JS	F2 JT	F2 JU	F2 JV	F2 JW	F2 JX	F2 JY	F2 JZ	F2 KA	F2 KB	F2 KC	F2 KD	F2 KE	F2 KF	F2 KG	F2 KH	F2 KI	F2 KJ	F2 KK	F2 KL	F2 KM	F2 KN	F2 KO	F2 KP	F2 KQ	F2 KR	F2 KS	F2 KT	F2 KU	F2 KV	F2 KW	F2 KX	F2 KY	F2 KZ	F2 LA	F2 LB	F2 LC	F2 LD	F2 LE	F2 LF	F2 LG	F2 LH	F2 LI	F2 LJ	F2 LK	F2 LL	F2 LM	F2 LN	F2 LO	F2 LP	F2 LQ	F2 LR	F2 LS	F2 LT	F2 LU	F2 LV	F2 LW	F2 LX	F2 LY	F2 LZ	F2 MA	F2 MB	F2 MC	F2 MD	F2 ME	F2 MF	F2 MG	F2 MH	F2 MI	F2 MJ	F2 MK	F2 ML	F2 MM	F2 MN	F2 MO	F2 MP	F2 MQ	F2 MR	F2 MS	F2 MT	F2 MU	F2 MV	F2 MW	F2 MX	F2 MY	F2 MZ	F2 NA	F2 NB	F2 NC	F2 ND	F2 NE	F2 NF	F2 NG	F2 NH	F2 NI	F2 NJ	F2 NK	F2 NL	F2 NM	F2 NN	F2 NO	F2 NP	F2 NQ	F2 NR	F2 NS	F2 NT	F2 NU	F2 NV	F2 NW	F2 NX	F2 NY	F2 NZ	F2 OA	F2 OB	F2 OC	F2 OD	F2 OE	F2 OF	F2 OG	F2 OH	F2 OI	F2 OJ	F2 OK	F2 OL	F2 OM	F2 ON	F2 OO	F2 OP	F2 OQ	F2 OR	F2 OS	F2 OT	F2 OU	F2 OV	F2 OW	F2 OX	F2 OY	F2 OZ	F2 PA	F2 PB	F2 PC	F2 PD	F2 PE	F2 PF	F2 PG	F2 PH	F2 PI	F2 PJ	F2 PK	F2 PL	F2 PM	F2 PN	F2 PO	F2 PP	F2 PQ	F2 PR	F2 PS	F2 PT	F2 PU	F2 PV	F2 PW	F2 PX	F2 PY	F2 PZ	F2 QA	F2 QB	F2 QC	F2 QD	F2 QE	F2 QF	F2 QG	F2 QH	F2 QI	F2 QJ	F2 QK	F2 QL	F2 QM	F2 QN	F2 QO	F2 QP	F2 QQ	F2 QR	F2 QS	F2 QT	F2 QU	F2 QV	F2 QW	F2 QX	F2 QY	F2 QZ	F2 RA	F2 RB	F2 RC	F2 RD	F2 RE	F2 RF	F2 RG	F2 RH	F2 RI	F2 RJ	F2 RK	F2 RL	F2 RM	F2 RN	F2 RO	F2 RP	F2 RQ	F2 RR	F2 RS	F2 RT	F2 RU	F2 RV	F2 RW	F2 RX	F2 RY	F2 RZ	F2 SA	F2 SB	F2 SC	F2 SD	F2 SE	F2 SF	F2 SG	F2 SH	F2 SI	F2 SJ	F2 SK	F2 SL	F2 SM	F2 SN	F2 SO	F2 SP	F2 SQ	F2 SR	F2 SS	F2 ST	F2 SU	F2 SV	F2 SW	F2 SX	F2 SY	F2 SZ	F2 TA	F2 TB	F2 TC	F2 TD	F2 TE	F2 TF	F2 TG	F2 TH	F2 TI	F2 TJ	F2 TK	F2 TL	F2 TM	F2 TN	F2 TO	F2 TP	F2 TQ	F2 TR	F2 TS	F2 TT	F2 TU	F2 TV	F2 TW	F2 TX	F2 TY	F2 TZ	F2 UA	F2 UB	F2 UC	F2 UD	F2 UE	F2 UF	F2 UG	F2 UH	F2 UI	F2 UJ	F2 UK	F2 UL	F2 UM	F2 UN	F2 UO	F2 UP	F2 UQ	F2 UR	F2 US	F2 UT	F2 UU	F2 UV	F2 UW	F2 UX	F2 UY	F2 UZ	F2 VA	F2 VB	F2 VC	F2 VD	F2 VE	F2 VF	F2 VG	F2 VH	F2 VI	F2 VJ	F2 VK	F2 VL	F2 VM	F2 VN	F2 VO	F2 VP	F2 VQ	F2 VR	F2 VS	F2 VT	F2 VU	F2 VV	F2 VW	F2 VX	F2 VY	F2 VZ	F2 WA	F2 WB	F2 WC	F2 WD	F2 WE	F2 WF	F2 WG	F2 WH	F2 WI	F2 WJ	F2 WK	F2 WL	F2 WM	F2 WN	F2 WO	F2 WP	F2 WQ	F2 WR	F2 WS	F2 WT	F2 WU	F2 WV	F2 WW	F2 WX	F2 WY	F2 WZ	F2 XA	F2 XB	F2 XC	F2 XD	F2 XE	F2 XF	F2 XG	F2 XH	F2 XI	F2 XJ	F2 XK	F2 XL	F2 XM	F2 XN	F2 XO	F2 XP	F2 XQ	F2 XR	F2 XS	F2 XT	F2 XU	F2 XV	F2 XW	F2 XX	F2 XY	F2 XZ	F2 YA	F2 YB	F2 YC	F2 YD	F2 YE	F2 YF	F2 YG	F2 YH	F2 YI	F2 YJ	F2 YK	F2 YL	F2 YM	F2 YN	F2 YO	F2 YP	F2 YQ	F2 YR	F2 YS	F2 YT	F2 YU	F2 YV	F2 YW	F2 YX	F2 YY	F2 YZ	F2 ZA	F2 ZB	F2 ZC	F2 ZD	F2 ZE	F2 ZF	F2 ZG	F2 ZH	F2 ZI	F2 ZJ	F2 ZK	F2 ZL	F2 ZM	F2 ZN	F2 ZO	F2 ZP	F2 ZQ	F2 ZR	F2 ZS	F2 ZT	F2 ZU	F2 ZV	F2 ZW	F2 ZX	F2 ZY	F2 ZZ
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Fig. 10B



1100

Name	Color	Score	Name	Color	Score	Name	Color	Score	Name	Color	Score
Sheet # DEMO1			Sheet # DEMO1			Sheet # DEMO2			Sheet # DEMO3		
Cluster Col A			Cluster Col B			Cluster Col C			Cluster Col		
Color	Score		Color	Score		Color	Score		Color	Score	
100	1		100	1		100	0		100	0	
Yellow			Yellow			Yellow			Yellow		
Columns FJ			Columns FJ			Columns			Columns		
Columns FJ			Columns FJ			Columns			Columns		
Name acids			Name amines			Name			Name		
Sheet # DEMO2			Sheet # DEMO3			Sheet # DEMO3			Sheet # DEMO3		
Cluster Col B			Cluster Col C			Cluster Col			Cluster Col		
Color	Score		Color	Score		Color	Score		Color	Score	
100	0		100	0		100	0		100	0	
Yellow			Yellow			Yellow			Yellow		
Columns FJ			Columns FJ			Columns			Columns		
Columns FJ			Columns FJ			Columns			Columns		

HELP

If you specify
name then the
column is a row
here, the weight
will apply to EACH
of the columns

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III: To quickly navigate among the worksheets in your workbook, especially if you have a lot of them, RIGHT-click on any of the tab-scrolling arrow buttons at the lower left of the screen, to get a list of sheet names to pick from.

Other shortcuts (see also the PANDORA manual):
Ctrl-Shift-J goes to the Append Control

III: To capture the name of a sheet for an entry into one of the control panels, double-click the sheet's tab to get a "Rename Sheet" dialog box. Then hit CTRL-C to Edit: Copy the name to the clipboard, and click Cancel on the Rename box. Go to the cell where you want to paste the sheet name, and either hit CTRL-V or do an Edit: Paste.

Cluster Control A

Fig. 11A

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Fig. 11B



1100			
Name		acids	
Sheet #		DEMO 2	
Cluster Col		B	
Color		Score	
red		0	
yellow		2	
Column(s)		Rel. Weight	
D		1	

Fig. 11C

Fig. 11C



Fig. 11D

1102	Name:	Canol
1104	Sheet #	DEMO 1
1104	Cluster Col	A
1112	Color	Score
1112	red	1
1112	yellow	1
1108	Relative Sort Order	
1108	Column (b)	Rel. Weight
1108	C/D	1
1108	E	1
1118	Columns	F1

1120



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B1		acid																	
name	acid	active group	activity @ 1 unit																
E1A	E1	A																	
E1B	E1	B	40																
E1C	E1	C	40																
E1D	E1	D																	
E2A	E2	A	7																
E2B	E2	B																	
E2C	E2	C	40																
E2D	E2	D																	
E3A	E3	A																	
E3B	E3	B																	
E3C	E3	C																	
E3D	E3	D																	
E4A	E4	A																	
E4B	E4	B																	
E4C	E4	C																	
E4D	E4	D																	
E5A	E5	A																	
E5B	E5	B																	
E5C	E5	C																	
E5D	E5	D	10																
E6A	E6	A																	

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Fig. 12



CMFD ID	# of replicates	S #	#PTS Test1	IC50 (nM) Test1	DATE Test1	#PTS Test2	IC50 (nM) Test2	DATE Test2	SELECT MITY
1-Dehtatocaine				no effect, 10000	7/20/97	4	884	4/10/97	
1-Dehtatocaine				no effect, 10000	7/20/97	4	>10000 (blank)	4/10/97	
1-Dehtatocaine				168.1333333	7/20/97	4	313	36330	0.00
0277				168.1333333	3/6/97	3	(blank) 10000	36498	0.00
0278				no effect	4/28/97	3	3575	35498	38.21
0629				no effect	10/9/97				
0631				168.5555557	3/6/97	3	4100	34997	15.59
0637				no effect	10/6/97				
0730				no effect	4/17/97	4	2885	36539.85714	679.87
0958				no effect	8/13/97	5	1283	8/18/97	32.08
1068				no effect	6/18/97	4	4000	6/23/97	8.39
10817-018-C				no effect	1/22/98				
1210				no effect	6/19/97	6	75000	6/24/97	2083.23
1329				no effect	8/13/97	5	23151	8/18/97	1158.05
1336				no effect	8/6/97	5	32303	8/7/97	310.41
1337				>300	8/14/97	5	43105	8/20/97	
1338				no effect	9/6/97	5	>100000	8/7/97	
1339				no effect	8/14/97	5	85442	8/19/97	291.81
1341				no effect	8/14/97	5	>100000	8/19/97	
1342				141	8/6/97	5	34184	8/7/97	242.44
1343				149	7/29/97	5	62285	7/31/97	418.09
1344				146	7/25/97	5	5080	7/30/97	35.03
1352				>300	7/19/97	4	63000	7/29/97	235.56
1353				>300	7/19/97	4	no effect	7/29/97	
1420				111	8/13/97	5	4537	8/18/97	41.35
1431				no effect	7/26/97	5	15367	7/30/97	
1433				no effect	8/14/97	5	no effect	8/20/97	
1444				no effect	8/14/97	5	>100000	8/20/97	
1445				no effect	10/8/97				
1446				no effect	8/14/97	5	no effect	8/20/97	
1447				no effect	10/8/97				
1453				>300	7/23/97	5	15494	7/30/97	463.21
1454				no effect	10/23/97				
1455				no effect	10/9/97				
1456				no effect	8/19/97	5	>100000	8/21/97	
1457				no effect	9/19/97				



CMPD ID	# of replicates	#PTS Test1	IC50 (nM) Test1	DATE Test1	#PTS Test2	IC50 (nM) Test2	DATE Test2	SELECT MTRY
5533			134	6/20/97	4	11000	6/25/97	82.05
5281				6/20/97	5	5000	6/25/97	171.43
6478				9/17/97	5	2650	9/16/97	49.28
6573			> 300	9/4/97	5	2486	9/11/97	
6741				9/17/97	5	1330	9/16/97	23.76
6530				6/18/97	5	10000	6/23/97	1000.00
7077			> 300	6/18/97	4	> 100000	6/23/97	
7339				10/6/97				
7368			> 10000	6/12/97	4	419	4/10/97	
7781			82	6/26/97	5	19000	7/3/97	231.71
7946			63	6/12/97	5	200	12/7/97	3.17
8374			185	7/27/97	5	2705	7/16/97	14.53
8437				9/25/97				
8503			no effect	8/19/97	5	> 100000	8/21/97	
8516				8/13/97	5	1872	8/18/97	31.73
8517				8/13/97	5	2836	8/18/97	72.72
8671			> 300	7/23/97	5	35852	7/31/97	
8826			> 300	9/18/97	5	no effect	9/16/97	
8857				9/4/97	5	3233	9/9/97	16.18
8858			no effect	9/4/97	5	9480	9/9/97	
8880			no effect	7/28/97	5	10630	9/9/97	
9116			108	8/13/97	5	16000	7/10/97	150.94
9176				8/13/97	5	2013	8/18/97	45.75
9177				8/13/97	5	1168	8/18/97	83.43
9202			no effect	9/2/97	5	3143	9/9/97	
9386				1/22/98				0.00
9657			> 300	10/3/97				
9751				11/14/97	5	1880	11/19/97	82.53
9940				10/8/97				
DE-EAS			no effect	8/24/97	5	no effect (blank)	8/20/97	
DTG			> 10000	2/5/97	5	21350	2/2/97	
Haloperidol				6/12/97	5	800	2/6/97	1.11
FPBP				9/17/97	5	3570	9/16/97	123.10
PPP			> 10000	3/7/97	5	75170	2/6/97	
propenone			no effect (10000)	8/24/97	5	no effect (blank)	8/20/97	
propenone				8/24/97	5	[blank] no effect	8/20/97	0.00

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Fig. 13B

CMFD ID	# of replicates	S #	#PTS Test1	IC50 (nM) Test1	DATE Test1	#PTS Test2	IC50 (nM) Test2	DATE Test2	SELECT MTY
(+)pentamidine				no effect	10000	7/20/97	4	6394	4/10/97
(-)pentamidine				no effect	10000	7/20/97	4	> 10000 (blank)	4/10/97
(+)pentamidine				no effect	10000	7/20/97	4	3153	355.50
(-)pentamidine				no effect	10000	7/20/97	4	3153	355.50
0277				158.5333333	366/97	3	(blank) 10000	354.98	0.00
0278				no effect	4/2/97	3	3576	354.98	38.21
0629				no effect	10/9/97				
0661				158.5333333	366/97	3	4100	399/97	15.59
0697				no effect	10/6/97				
0793				no effect	4/17/97	4280714286	26885	35533.65714	679.87
0858				no effect	8/13/97	5	1283	8/18/97	32.08
1058				no effect	6/18/97	4	4000	6/23/97	8.59
10817-018-C				no effect	1/22/98				
1210									
1229									
1266									
1317									
1337									
1338									
1339									
1341									
1342									
1343									
1344									
1362									
1389									
1420									
1431									
1439									
1444									
1445									
1446									
1447									
1453									
1463									
1464									
1465									
1466									
1467									

ENTER SCALING FACTOR FOR DISPLAY

> 300	7/11/97	4	6394	7/20/97	41.95
11	8/13/97	5	4687	8/18/97	
no effect	7/20/97	5	1687	7/30/97	
no effect	8/14/97	5	no effect	9/20/97	
no effect	8/14/97	5	> 100000	8/20/97	
no effect	10/8/97				
no effect	8/14/97	5	no effect	8/20/97	
no effect	10/8/97				
no effect	7/20/97	5	15464	7/30/97	469.21
> 300	9/25/97				
no effect	10/2/97				
no effect	10/8/97				
no effect	8/18/97	5	> 100000	9/21/87	
no effect	9/18/97				

Fig. 13C

Fig. 13D

1. The following information is being furnished to you by the Department of the Treasury, Internal Revenue Service, for your information:

	Oignd	Series	Test1	Test2	Test3	HTS SPA Dose-Resp X Inhib @ 3 μM	HTS SPA Dose-Resp X Inhib @ 1 μM	HTS SPA Dose-Resp X Inhib @ 0.3 μM	HTS SPA Dose-Resp X Inhib @ 0.1 μM
1									
2	Cmpd01	N							
3	Cmpd02	N							
4	Cmpd03	G							
5	Cmpd04	N							
6	Cmpd05	N							
7	Cmpd06	D							
8	Cmpd07	D							
9	Cmpd08	D							
10	Cmpd09	D							
11	Cmpd10	N	0.23						
12	Cmpd11	N	1						
13	Cmpd12	H	1						
14	Cmpd13	H	1.2						
15	Cmpd14	H	0.8						
16	Cmpd15	H	0.39						
17	Cmpd16	I							
18	Cmpd17	K							
19	Cmpd18	I	5.31						
20	Cmpd19	I	0.13						
21	Cmpd20	F							
22	Cmpd21	K							
23	Cmpd22	B							
24	Cmpd23	B							
25	Cmpd24	B							
26	Cmpd25	B							
27	Cmpd26	B	0.89						
28	Cmpd27	B	0.111						
29	Cmpd28	E							

SCORING OF UNCOLORED CELLS

RANDOMLY SELECTED UNCOLORED CELLS ARE USED TO DETERMINE THE PERCENTAGE OF UNCOLORED CELLS.

USE THIS IS A RECOMMENDATION FOR THE USE OF THIS SOFTWARE.

THIS IS A RECOMMENDATION FOR THE USE OF THIS SOFTWARE. IT IS NOT A GUARANTEE OF PERFORMANCE OR RESULTS.

WARNING: This software is not intended for use as a diagnostic tool or for medical purposes.

This software is not intended for use as a diagnostic tool or for medical purposes. It is not a guarantee of performance or results.

Fig. 14A

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Cmpd	Series	Test1	Test2	Test3	HTS SPA Dose-Resp % Inhib @ 3x10 ⁻⁶ M	HTS SPA Dose-Resp % Inhib @ 1x10 ⁻⁵ M	HTS SPA Dose-Resp % Inhib @ 3x10 ⁻⁷ M	HTS SPA Dose-Resp % Inhib @ 1x10 ⁻⁷ M
Cmpd38	L				50			
Cmpd44	O				70			
Cmpd45	M				71			
Cmpd46	A		0.18	1.5x10 ⁻⁵			53	
Cmpd48	D			2.8	68			
Cmpd49	Q		0.56		68			
Cmpd51	H		0.117	4.5	69			
Cmpd52	D							
Cmpd57	H							
Cmpd58	H	0.28	0.41					
Cmpd61	H	0.355	0.148					
Cmpd65	B							
Cmpd69	F	0.58	0.41					
Cmpd72	F	0.58	0.9					
Cmpd47	F							
Cmpd50	F							
Cmpd51	Q							
Cmpd57	A							
Cmpd59	D	0.119						
Cmpd61	N	0.23						
Cmpd62	H		0.24					
Cmpd69	I	0.134						
Cmpd70	F		0.317					
Cmpd72	B		0.16					
Cmpd74	B		0.27					
Cmpd75	B	0.853			71		58	
Cmpd76	B	0.111			70		53	
Cmpd78	E		0.13				1	
Cmpd79	J		0.46				1	
Cmpd81	J	0.63					1	
Cmpd85	J		0.22				3	
Cmpd86	Q	0.258					18	
Cmpd87	H		0.13				18	
Cmpd88	F	0.5					4	

Fig. 14B

Fig. 14C

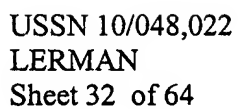
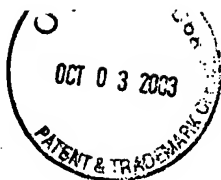


Fig. 14D



cluster label	# of compds (unlocked)	score		Scoring of sheet DEMO 2 using parameter set "acids"																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																				</
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Fig. 15A

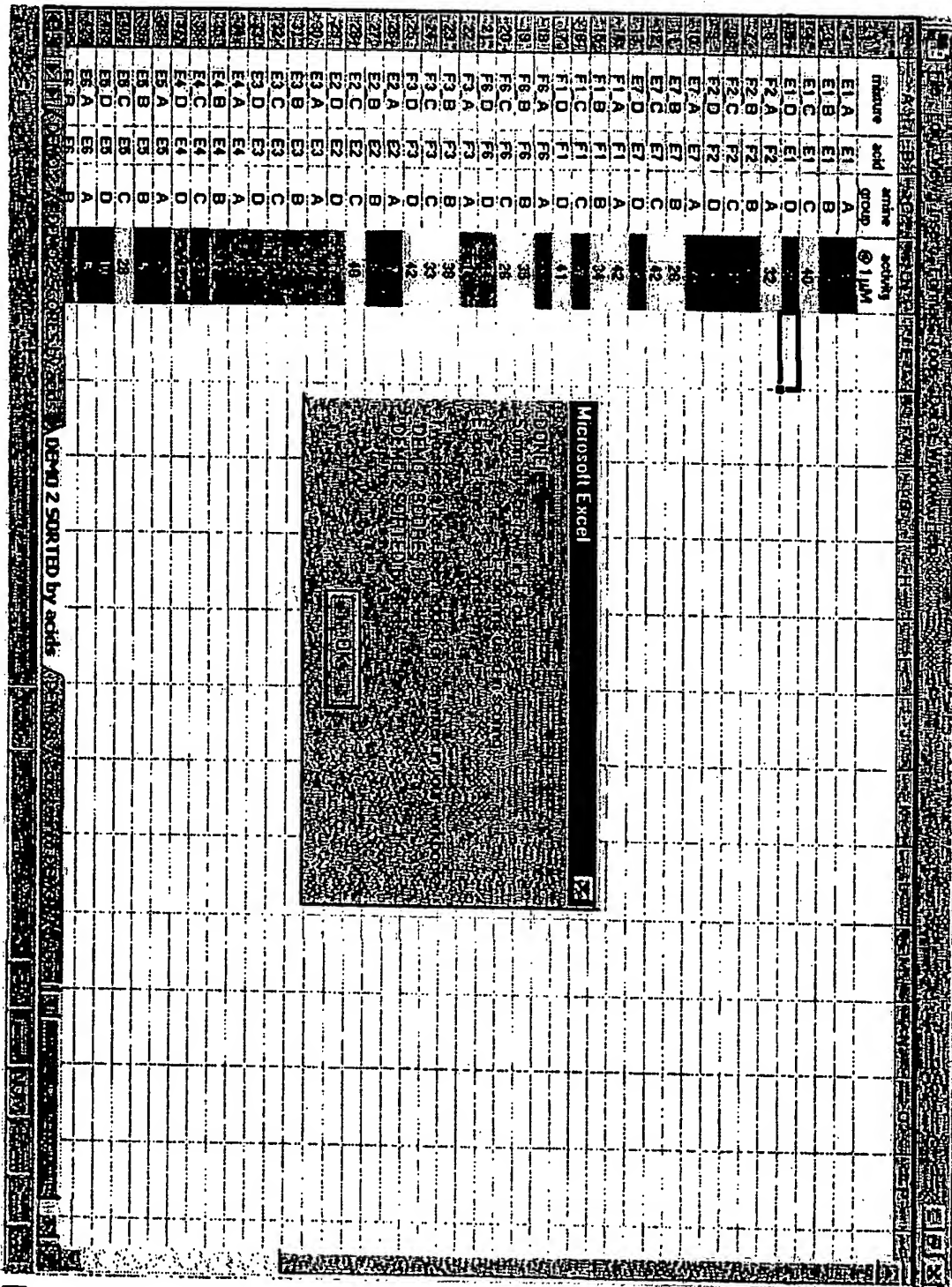


Fig. 15B



A	B	C	D	E
Cmpd	HTS SPA Dose-Resp % Inhib @ 3x10-6M	HTS SPA Dose-Resp % Inhib @ 1x10-6M	HTS SPA Dose-Resp % Inhib @ 3x10-7M	HTS SPA Dose-Resp % Inhib @ 1x10-7M
1				
2	Cmpd01	22	16	13
3	Cmpd02	41	22	5
4	Cmpd03	57	28	15
5	Cmpd04	25	24	29
6	Cmpd05	60	21	22
7	Cmpd06	41	13	3
8	Cmpd07	28	48	43
9	Cmpd08	28	28	38
10	Cmpd09	41	22	15
11	Cmpd10	42	24	5
12	Cmpd11	50	53	25
13	Cmpd12	25	24	3
14	Cmpd13	23	40	37
15	Cmpd14	39	4	12
16	Cmpd15	1146	46	35
17	Cmpd16	64	38	18
18	Cmpd17	64	47	24
19	Cmpd18	54	22	32
20	Cmpd19		20	12
21	Cmpd20			

Figure 16A



Click here to download	
sheet	DEMO 1
column(s)	B:E
# of colors	
break 1	33
break 2	67
break 3	
color 1	red
color 2	yellow
color 3	
Re-scale all?	

Figure 16B



A	B	C	D	E	F	G	H
Cmpd	HTS SPA Dose-Resp % Inhib @ 3x10-6M 3.00e-06	HTS SPA Dose-Resp % Inhib @ 1x10-6M 1.00e-06	HTS SPA Dose-Resp % Inhib @ 3x10-7M 3.00e-07	HTS SPA Dose-Resp % Inhib @ 1x10-7M 1.00e-07	D-R -iveness score (0 to 100) by Cmpd	D-R activity score (0 to 100) by Cmpd	D-R composite score (0 to 100) by Cmpd
1							
2	Cmpd20	100	100	100	75	100	100
3	Cmpd07	100	42	48	83	77	79
4	Cmpd13	50	59	40	83	70	75
5	Cmpd15	50	46	46	83	70	75
6	Cmpd16	100	64	38	92	50	70
7	Cmpd17	50	64	47	92	43	67
8	Cmpd03	50	57	28	92	23	57
9	Cmpd05	50	60	21	92	23	57
10	Cmpd06	50	41	13	92	23	57
11	Cmpd09	50	41	22	92	23	57
12	Cmpd11	50	77	22	67	47	57
13	Cmpd18	50	54	22	92	23	57
14	Cmpd19	50	71	23	83	30	56
15	Cmpd10	61	42	24	83	20	51
16	Cmpd01	50	22	16	83	10	46
17	Cmpd04	50	25	24	83	10	46
18	Cmpd02	41	3	22	83	7	45
19	Cmpd08	50	3	22	58	33	45
20	Cmpd12	47	25	24	83	7	45
21	Cmpd14	38	23	4	83	7	45

Fig. 16C



A	B	C	D	E	F	G	H
cmpd	HTS SPA Dose-Resp % Inhib @ 3x10-6M 3.00e-06	HTS SPA Dose-Resp % Inhib @ 1x10-6M 1.00e-06	HTS SPA Dose-Resp % Inhib @ 3x10-7M 3.00e-07	HTS SPA Dose-Resp % Inhib @ 1x10-7M 1.00e-07	D-R -iveness score by cmpd	D-R activity score by cmpd	D-R composite score by cmpd
1							
22	marker_7.5				75	100	100
23	marker_7.0				83	87	86
24	marker_6.5				92	50	70
25	marker_6.0		50/117	49	92	23	57
26	marker_5.5	49	24	9	83	7	45
27	marker_5.0	23	9	3	75	0	38

Figure 16D



A	B	C	D	E	F	G	H	I	J
Cmpd	HTS SPA Dose-Resp % Inhib @ 3x10-6M 3.00e-06	HTS SPA Dose-Resp % Inhib @ 1x10-6M 1.00e-06	HTS SPA Dose-Resp % Inhib @ 3x10-7M 3.00e-07	HTS SPA Dose-Resp % Inhib @ 1x10-7M 1.00e-07	D-R Aveness score (0 to 100) by Cmpd	D-R activity score (0 to 100) by Cmpd	D-R composite score (0 to 100) by Cmpd	Interp log IC50 by Cmpd	est IC50 μM by Cmpd
1									
2	Cmpd20	10	10	48	75	100	100		<0.1
3	marker_7.5	10	10	50	83	87	88		
4	marker_7.0	10	10	43	83	77	79	6.78	0.17
5	Cmpd07	59	46	40	83	70	75	6.66	0.22
6	Cmpd13	46	46	38	83	70	75	6.66	0.22
7	Cmpd15	11	11	49	92	50	70	6.50	0.32
8	Cmpd16	11	11	18	92	50	70		
9	marker_6.5	11	11	24	92	43	67	6.38	0.41
10	Cmpd17	64	57	47	92	23	57	6.00	1
11	Cmpd03	57	80	21	92	23	57	6.00	1
12	Cmpd05	41	41	13	92	23	57	6.00	1
13	Cmpd06	41	41	20	92	23	57	6.00	1
14	Cmpd09	50	54	63	67	47	57	6.00	1
15	Cmpd11	50	54	21	92	23	57	6.00	1
16	Cmpd18	50	54	21	92	23	57	6.00	1
17	marker_6.0	50	54	21	92	23	57	6.00	1
18	Cmpd19	61	42	21	83	30	56	5.96	1.1
19	Cmpd10	61	42	21	83	20	51	5.75	1.8
20	Cmpd01	61	42	21	83	10	46	5.54	2.9
21	Cmpd04	41	35	21	83	10	46	5.54	2.9
22	Cmpd02	41	35	21	83	7	45		>3
23	Cmpd08	66	58	28	58	33	45		>3
24	Cmpd12	47	35	22	83	7	45		>3
25	Cmpd14	39	23	4	83	7	45		>3
26	marker_5.5	49	24	9	83	7	45		>3
27	marker_5.0	23	9	3	75	0	38		

Figure 16E



Fig. 16F

The complete data set for 3 points and 3 colors, in systematic order.

compound	percent inhibition		data group number		data group color	
	highest conc	lowest conc	highest conc	lowest conc	highest conc	lowest conc
compd 01	2	29	1	1		
compd 02	16	10	1	1		
compd 03	31	26	1	1		
compd 04	21	46	1	2		
compd 05	30	53	1	2		
compd 06	17	37	1	2		
compd 07	26	90	1	3		
compd 08	10	90	1	3		
compd 09	32	72	1	3		
compd 10	34	17	1	1		
compd 11	51	8	2	1		
compd 12	56	3	2	1		
compd 13	33	39	2	2		
compd 14	53	52	2	2		
compd 15	51	62	2	2		
compd 16	85	82	2	3		
compd 17	43	71	2	3		
compd 18	66	99	2	3		
compd 19	87	11	3	1		
compd 20	87	5	3	1		
compd 21	77	8	3	1		
compd 22	78	36	3	2		
compd 23	85	40	3	2		
compd 24	83	57	3	3		
compd 25	73	88	3	3		
compd 26	69	85	3	3		
compd 27	79	68	3	3		

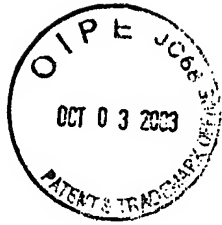


Fig. 166

The complete data set for 3 points and 3 colors, sorted by decreasing dose-responsiveness

compound	highest conc	lowest conc	step scoring	unscaled score points	scaled responsiveness 0-100
compd 22			+1+1	2	100
compd 10			+1+0	1	88
compd 13			+1+0	1	88
compd 19			+1+0	1	88
compd 23			+1+0	1	88
compd 25			+1+0	1	88
compd 26			+1+0	1	88
compd 01			+1+0	1	88
compd 14			+1+0	1	88
compd 27			+1+0	1	88
compd 04			+1+0	1	88
compd 07			+1+0	1	88
compd 08			+1+0	1	88
compd 11			+1+0	1	88
compd 12			+1+0	1	88
compd 18			+1+0	1	88
compd 17			+1+0	1	88
compd 20			+1+0	1	88
compd 21			+1+0	1	88
compd 24			+1+0	1	88
compd 02			+1+0	1	88
compd 03			+1+0	1	88
compd 05			+1+0	1	88
compd 09			+1+0	1	88
compd 15			+1+0	1	88
compd 16			+1+0	1	88
compd 18			+1+0	1	88
compd 06			+1+0	1	88

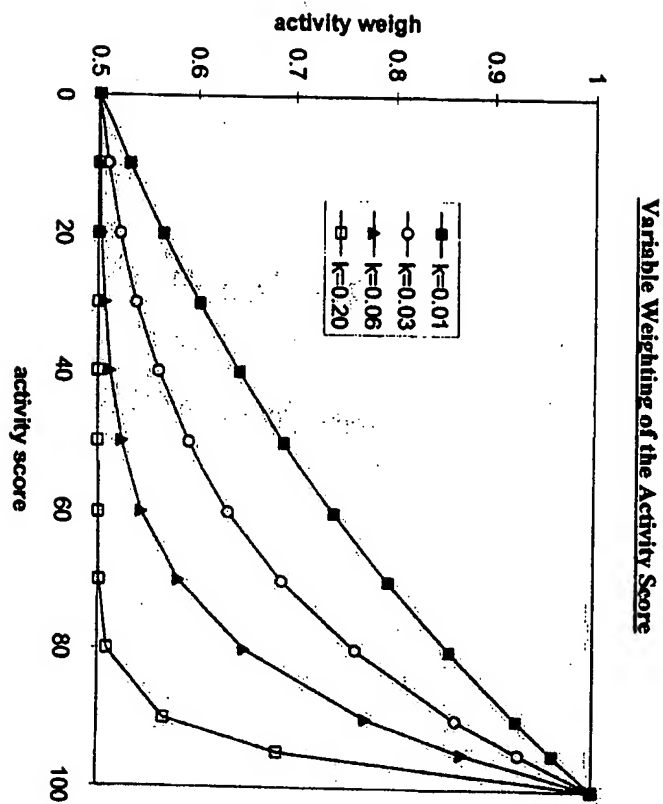


Fig. 16H

The complete set of data for 3 points and 3 colors, sorted by decreasing overall activity.

compound	data group number			data group color			activity scoring	unscaled activity points	scaled activity 0-100
	highest conc	→	lowest conc	highest conc	→	lowest conc			
compd 27	3	3	3				1(3)+2(3)+3(3)	18	100
compd 18	2	3	3				1(2)+2(3)+3(3)	17	92
compd 24	3	2	2				1(3)+2(2)+3(3)	16	83
compd 09	1	3	3				1(1)+2(3)+3(3)	16	83
compd 26	3	3	2				1(3)+2(3)+3(2)	15	75
compd 16	2	2	3				1(2)+2(2)+3(3)	15	75
compd 17	2	3	2				1(2)+2(3)+3(2)	14	67
compd 21	3	1	3				1(3)+2(1)+3(3)	14	67
compd 06	1	2	3				1(1)+2(2)+3(3)	14	67
compd 23	3	3	2				1(3)+2(2)+3(2)	13	58
compd 08	1	2	3				1(1)+2(3)+3(1)	13	58
compd 12	2	3	1				1(2)+2(1)+3(3)	13	58
compd 25	3	2	3				1(3)+2(2)+3(1)	12	50
compd 03	2	2	1				1(2)+2(3)+3(1)	12	50
compd 14	1	3	3				1(1)+2(1)+3(3)	12	50
compd 03	2	3	1				1(2)+2(3)+3(1)	11	42
compd 16	1	2	2				1(3)+2(1)+3(2)	11	42
compd 20	3	3	1				1(1)+2(2)+3(2)	11	42
compd 05	1	2	2				1(3)+2(2)+3(1)	10	33
compd 07	3	3	1				1(1)+2(3)+3(1)	10	33
compd 11	2	1	2				1(2)+2(1)+3(2)	10	33
compd 13	1	2	1				1(3)+2(2)+3(1)	9	25
compd 02	2	1	2				1(1)+2(1)+3(2)	9	25
compd 19	3	1	1				1(3)+2(1)+3(1)	8	17
compd 04	1	2	1				1(1)+2(2)+3(1)	7	8
compd 10	2	1	1				1(2)+2(1)+3(1)	6	0
compd 01	1	1	1				1(1)+2(1)+3(1)	6	0

Fig. 16I



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Fig. 16J

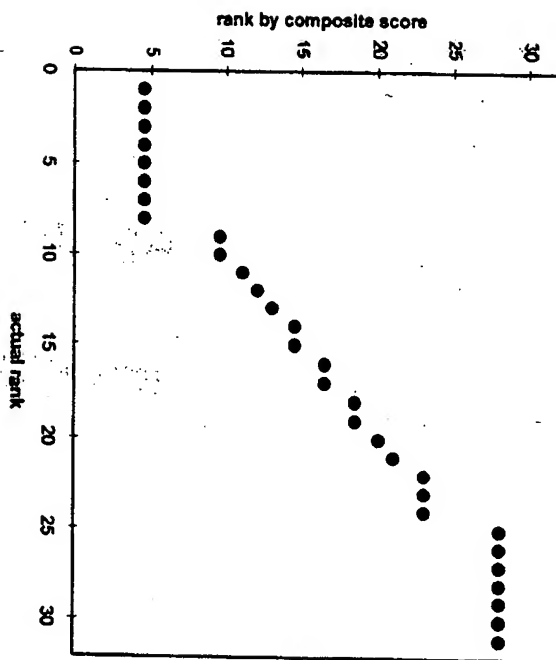
The complete set of data for 3 points and 3 colors, sorted by decreasing composite score.

compound	highest conc	lowest conc	scaled responsive-ness, 0-100	scaled activity 0-100	composite 0-100
compd 27			76	100	100
compd 18			38	92	82
compd 26			88	75	80
compd 24			50	83	72
compd 23			88	58	72
compd 09			38	83	68
compd 25			88	50	68
compd 22			100	33	68
compd 14			75	50	62
compd 15			38	75	61
compd 17			50	67	60
compd 21			50	67	60
compd 13			88	25	56
compd 08			50	58	54
compd 12			50	17	52
compd 19			88	8	48
compd 10			50	42	46
compd 16			50	42	46
compd 20			38	50	44
compd 03			50	33	41
compd 07			38	33	41
compd 11			50	33	41
compd 06			38	42	40
compd 05			0	67	38
compd 08			75	0	38
compd 01			50	17	33
compd 04			38	25	31
compd 02					





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Quality of Ranking when Noise = 10 Inhibition Percentage Points

Fig. 16K

Fig. 16L

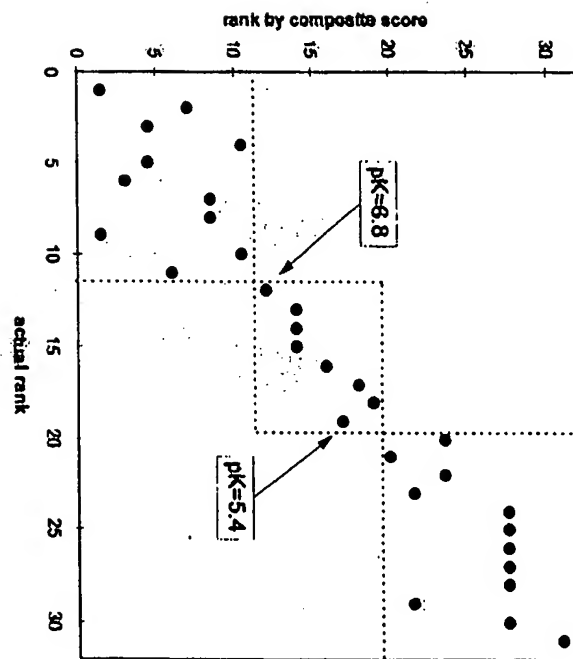




Fig. 16M

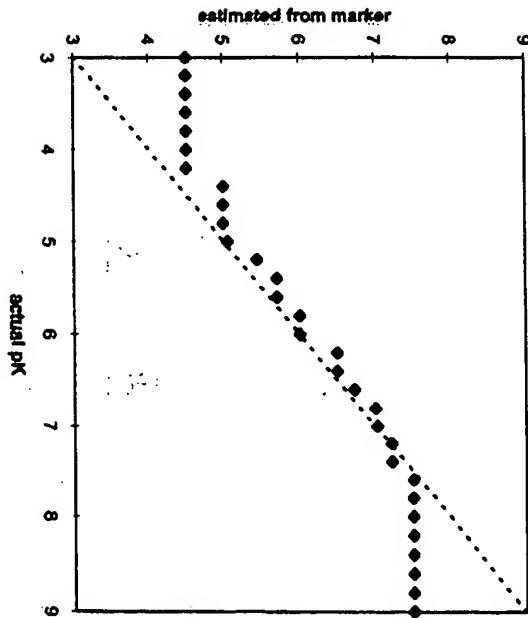
Quantitative Estimation of Potencies by Calibration Marker Compounds

compound	% inh @ 3.00e-06	% inh @ 1.00e-08	% inh @ 3.00e-07	% inh @ 1.00e-07	D.R. composite score	interp log IC50 /M	est IC50 /M
M33875	100	102	83	75	79		<0.1
marker 7.5	99	97	90	78	79		
M221211	110	91	69	39	78	7.00	0.10
M371585	108	102	63	27	76	7.00	0.10
marker 7.0	97	91	75	30	76		
M345077	102	87	92	87	75	6.97	0.11
M371796	91	78	76	33	73	6.90	0.13
M143629	100	79	48	43	69	6.77	0.17
M371890	101	72	42	29	69	6.77	0.17
M371891	92	69	55	49	69	6.77	0.17
M309032	105	62	62		67	6.70	0.20
M198289	101	82	38		66	6.67	0.22
M224602	97	79	43		66	6.67	0.22
M318671	93	63	42		66	6.67	0.22
M273373	95	83	52		65	6.63	0.23
M371336	78	70	44	27	62	6.53	0.29
M371825	61	64	60	26	62	6.53	0.29
M181250	99	46	46	25	61	6.50	0.32
M338331	87	73	29		61	6.50	0.32
marker 6.5	90	76	49	24	61		
M143630	65	28	28	38	60	6.44	0.36



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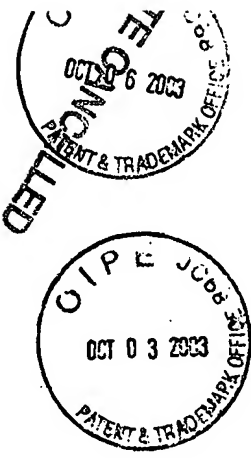
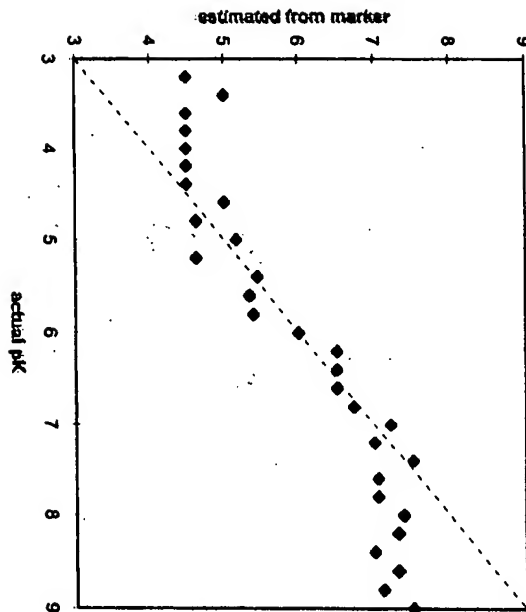


Quality of Estimation when Noise = 10 Inhibition Percentage Points

Fig. 16N

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Fig. 16P



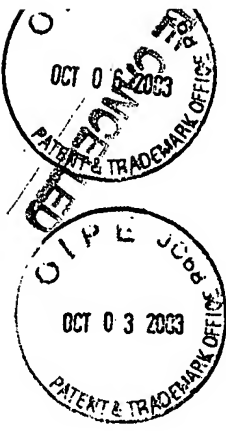
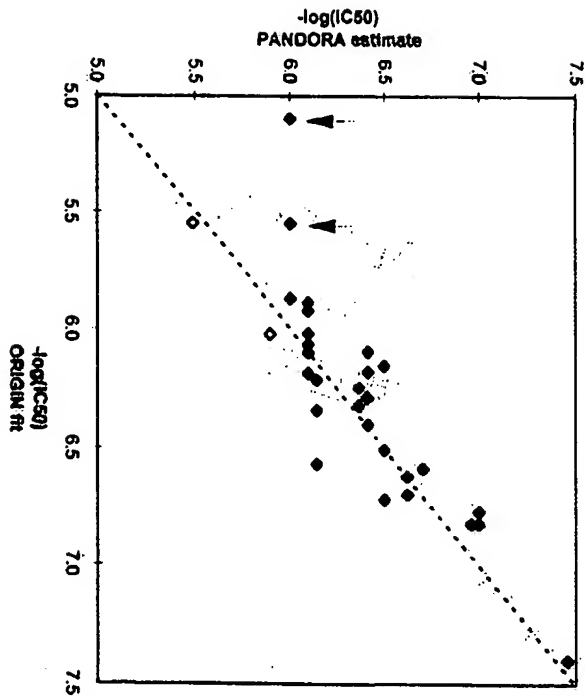


Fig. 16Q

Comparison of Curve Fitting to Marker Calibration
for T-cell Proliferation Data



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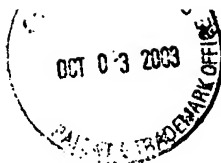
Compd	Series	Test1	Test2	Test3	HTS SPA			
					Dose-Resp % Inhib @ 3x10-6M	Dose-Resp % Inhib @ 1x10-6M	Dose-Resp % Inhib @ 3x10-7M	Dose-Resp % Inhib @ 1x10-7M
1	Compd01	N	29	30	41	3	22	5
2	Compd02	N	42	55	83	57	28	15
3	Compd03	G	261	11	70	25	24	29
4	Compd04	N	30	30	89	60	21	22
5	Compd05	N	1.8	9.2	71	41	13	3
6	Compd06	D	8.86	6.5	100	79	48	43
7	Compd07	D	3.11	0.037	65	28	28	38
8	Compd08	D	0.089	N.A.	68	41	22	15
9	Compd09	D	0.119		61	42	24	5
10	Compd10	N	0.233		50	77	63	25
11	Compd11	N	4.31		47	25	24	3
12	Compd12	H	1.3	0.24	81	59	40	37
13	Compd13	H	1.17	0.194	39	23	4	12
14	Compd14	H	0.26	0.41	99	46	46	36
15	Compd15	H	0.369	0.148	101	82	38	18
16	Compd16	K	0.87	30	79	54	22	32
17	Compd17	K	0.223	N.A.	71	71	23	12
18	Compd18		5.27		101	109	108	100
19	Compd19		0.134		87	70	31	13
20	Compd20		0.317		94	77	36	12
21	Compd21	K	2.21		96	61	36	12
22	Compd22	B	0.15		110	91	69	39
23	Compd23	B						
24	Compd24	B	3.487	0.27				

Figure 17A



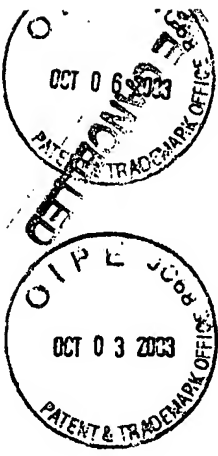
THIS COLORING INDICATES A DATA COLUMN WITH MIXED DATA TYPES												
orig col	heading	#	#	#	#	# total (longest col)	last occupied row num.	minimum (4 sig fig)	maximum (4 sig fig)	mean (4 sig fig)	standard dev (4 sig fig)	unique text strings and counts (24 different)
A	Unpd		24			24	25					B (3) D (4) G (1) H (4) K (2) N (6)
B	Series		20		4	24	25					
C	Test1	12		12	24	24	25	0.119	8.86	2.385	2.726	
D	Test2	17		7	24	24	25	0.037	42	5.122	11.77	
E	Test3	10	2	12	24	24	25	0.4	30	15.76	12.59	NA (2)
F	HTS SPA Dose-Resp % Inhib @ 3x10-6M	23			24	24	25	39	110	77.57	20.43	
G	HTS SPA Dose-Resp % Inhib @ 1x10-6M	23			24	24	25	3	109	55.87	25.24	
H	HTS SPA Dose-Resp % Inhib @ 3x10-7M	23			24	24	25	4	108	35.52	21.85	
I	HTS SPA Dose-Resp % Inhib @ 1x10-7M	23			24	24	25	3	100	23.91	20.74	

Figure 17B



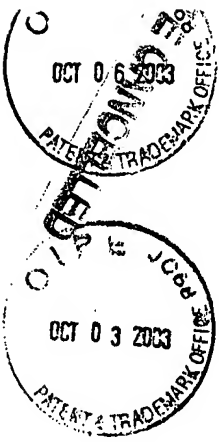
A	B	C	D	E	F	G
project name	most important factor scored by Mngt A	most important factor scored by Mngt B	most important factor scored by Mngt C	less important factor scored by Mngt A	less important factor scored by Mngt B	less important factor scored by Mngt C
1						
2 Proj 01	2		2	1	2	2
3 Proj 02	1	1	1	2	1	2
4 Proj 03	1	1		1	2	
5 Proj 04				1	2	1
6 Proj 05					1	2
7 Proj 06	2		1		2	1
8 Proj 07		1	1			1
9 Proj 08		1	2		1	
10 Proj 09			1		2	1
11 Proj 10	2	1		1		1
12 Proj 11	1	1	1	2	1	
13 Proj 12			1	1		2
14 Proj 13		1				2
15 Proj 14		2	2			
16 Proj 15	2		2	2	2	2
17 Proj 16	1	2	2	1	2	
18 Proj 17	2	1		2	2	2
19 Proj 18				1		
20 Proj 19	2	2	2		1	1
21 Proj 20		2		1		2

Figure 18A



Click here to run a test	
sheet	Portfolio
column(s)	B:G
# of colors	3
break 1	1
break 2	2
break 3	3
color 1	red
color 2	yellow
color 3	
Re-scale all?	

Figure 188



Name:		Factors
College Cluster		
Sheet #	Portfolio	
Cluster Col	A	
Serial Cluster		
Color	Score	
red	1	
yellow	2	
Score and Sort Elusters		
Columns	Rel. Weight	
B:D	3	
E:G	1	

Figure 18C

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A	B	C	D	E	F	G	H
project name	most important factor scored by Mngr A	most important factor scored by Mngr B	most important factor scored by Mngr C	less important factor scored by Mngr A	less important factor scored by Mngr B	less important factor scored by Mngr C	score (0-100)
1 Proj 18							94
2 Proj 05						2	92
3 Proj 04					2		86
4 Proj 14		2	2			1	83
5 Proj 20		2	2			2	83
6 Proj 13		2				2	81
7 Proj 09					2		75
8 Proj 12						2	75
9 Proj 15	2			2	2	2	75
10 Proj 01	2				2	2	72
11 Proj 08							69
12 Proj 06	2				2		67
13 Proj 17	2			2	2		67
14 Proj 19	2					2	64
15 Proj 07							61
16 Proj 03					2		58
17 Proj 10	2						58
18 Proj 16		2			2		58
19 Proj 02				2		2	39
20 Proj 11				2			36

Figure 18D

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Fig. 19
Drug Candidate Compounds;
Scored, Sorted, and Vertically Compressed

Compd	Cluster	CD45 HTS	IRP HTS	APOP HTS	ACC	DON	dLogP	NMW	HTS Selectivity Ratio	Ratio A/N _{um}	Pcrit Crt
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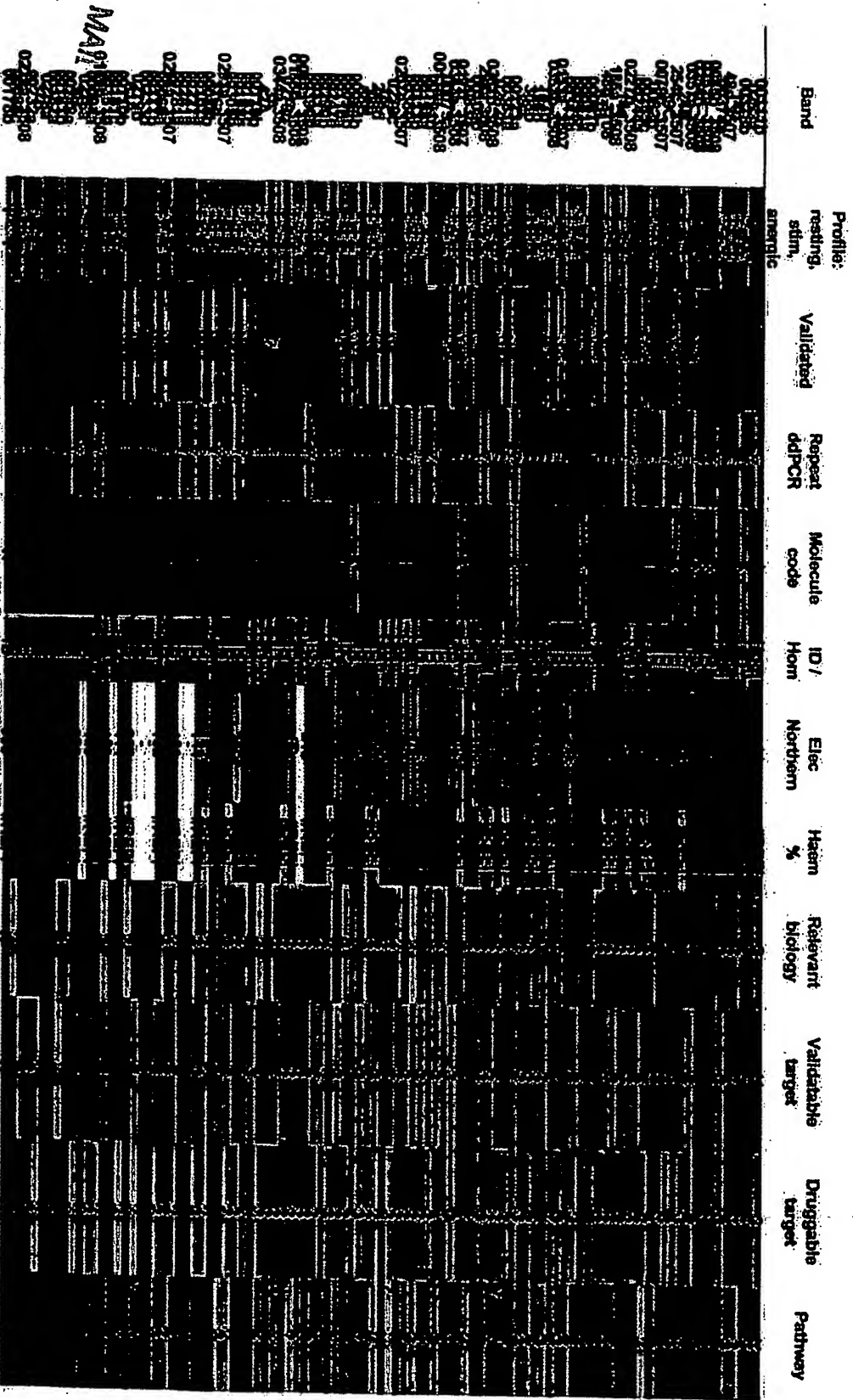


Fig. 20 Target Protein Candidates

MAIL D

Fig. 21

project name	most important factor scored by manager 1	most important factor scored by manager 2	most important factor scored by manager 3	less important factor scored by manager 1	less important factor scored by manager 2	less important factor scored by manager 3
Proj 18						
Proj 05						
Proj 04						
Proj 14						
Proj 20						
Proj 13						
Proj 09						
Proj 12						
Proj 15						
Proj 01						
Proj 08						
Proj 06						
Proj 17						
Proj 19						
Proj 07						
Proj 03						
Proj 10						
Proj 16						
Proj 02						
Proj 11						

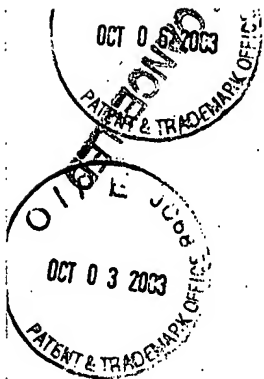
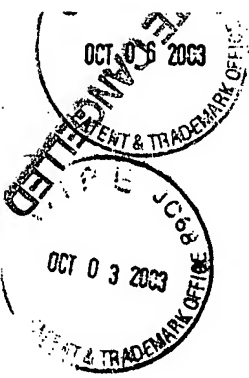


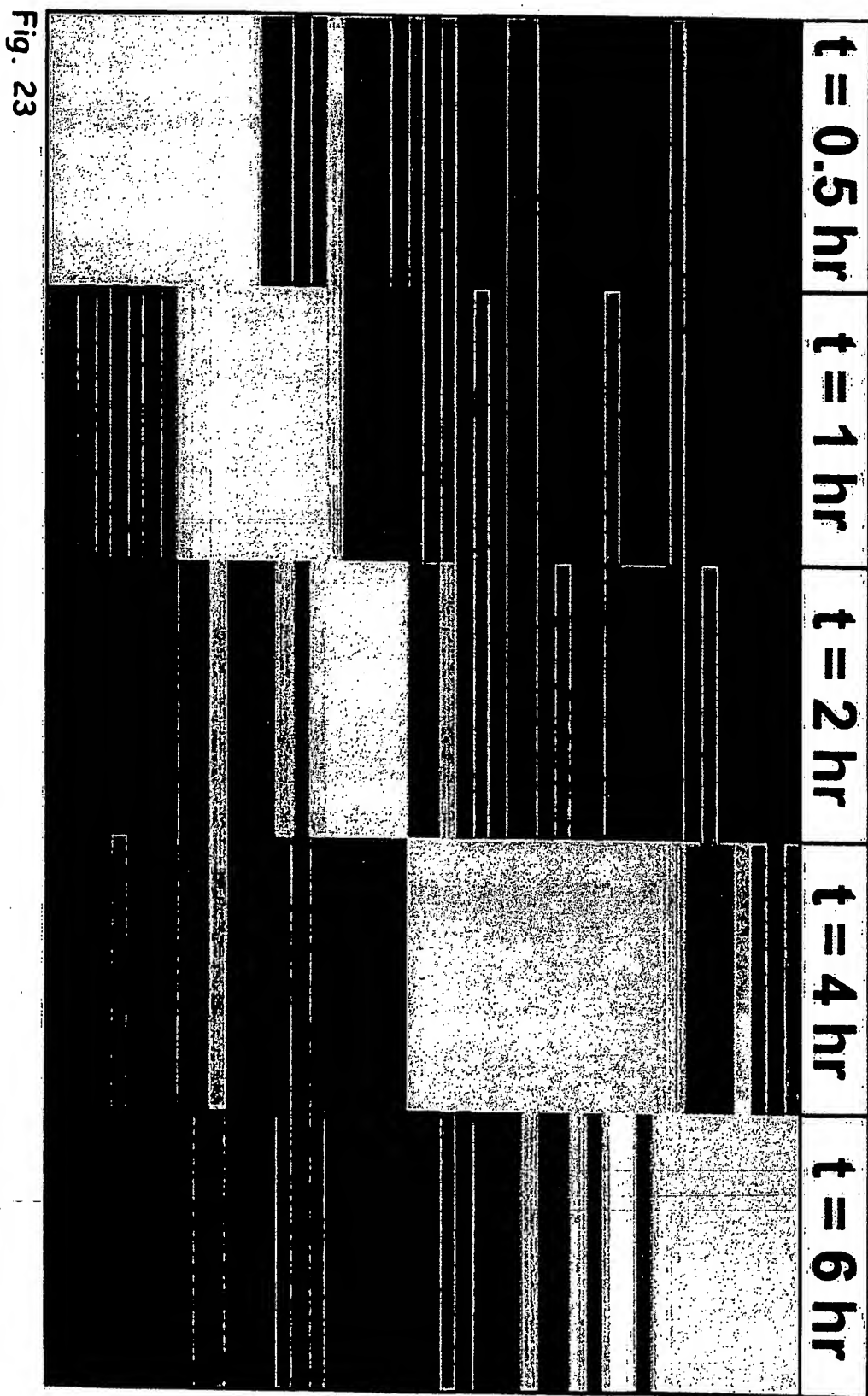
Fig. 22

Company	Disease 1	Disease 2	Disease 3	Disease 4	Disease 5	Disease 6	Disease 7	Disease 8	Disease 9	Disease 10	Disease 11	Disease 12
Company 1	Phase I				L/I/O			L/I/O	Phase I		Phase II	Phase I
Company 2	Phase I	LI	Phase II			L/I/O	L/I/O	L/I/O	Phase I	L/I/O		
Company 3	L/I/O				L/I/O	Phase II	L/I/O	Phase I				
Company 4					L/I/O	Phase II	L/I/O	Phase I				
Company 5	L/I/O			L/I/O	L/I/O	Phase II	L/I/O					TS/LI
Company 6												
Company 7	L/I/O							Phase I	L/I/O			LI
Company 8	L/I/O	Phase II			L/I/O			Phase I	L/I/O			
Company 9	L/I/O					Phase I	L/I/O	L/I/O	L/I/O			L/I/O
Company 10				L/I/O	Phase III					Phase I		
Company 11	L/I/O			L/I/O	L/I/O							
Company 12	L/I/O		Phase II		L/I/O							L/I/O
Company 13	LI				Phase III		Phase III					
Company 14	L/I/O		L/I/O		L/I/O		L/I/O	L/I/O				
Company 15	LI		LI	LI	LI		Phase II			LI		
Company 16	LI											
Company 17	Phase II				L/I/O	L/I/O						
Company 18							Phase I					
Company 19	LI		LI				LI					
Company 20				L/I/O								
Company 21	L/I/O				Phase III							
Company 22	TS		TS			TS				TS		
Company 23	LI				L/I/O							
Company 24	LI											
Company 25	L/I/O											



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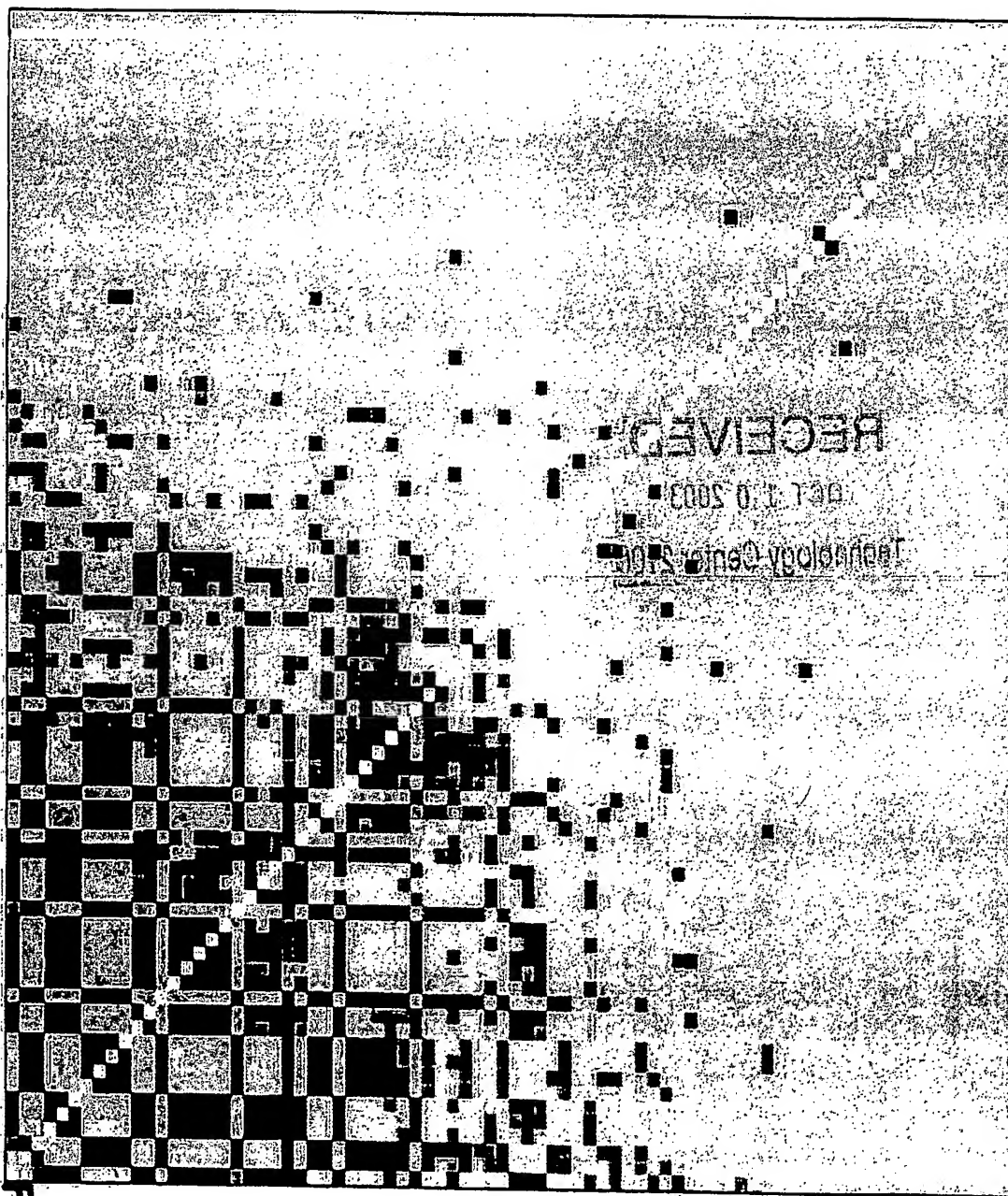


Fig. 24

